

Methyl 3,6-dichloropyridine-2-carboxylate

Other names:	Clopyralid acid, methyl ester Clopyralid, methyl ester
Inchi:	InChI=1S/C7H5Cl2NO2/c1-12-7(11)6-4(8)2-3-5(9)10-6/h2-3H,1H3
InchiKey:	HQTUEAOWLWJLF-UHFFFAOYSA-N
Formula:	C7H5Cl2NO2
SMILES:	COC(=O)c1nc(Cl)ccc1Cl
Mol. weight [g/mol]:	206.03
CAS:	1532-24-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	2.175		Crippen Method
mcvol	127.630	ml/mol	McGowan Method
rinpol	1413.00		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1413.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1532247&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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